

Benzoic acid, 2-methoxy-
579-75-9 | DTXSID3060376

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 279 °C

Global applicability domain: Inside

Local applicability domain index: 6.92e-01

Confidence level: 8.67e-01

Nearest Neighbors from the Training Set

Image not found

Benzoic acid, 4-methoxy-

Measured: 277

Predicted: 279

Image not found

Phenoxyacetic acid

Measured: 285

Predicted: 279

Image not found

Hydrocinnamic acid

Measured: 280

Predicted: 270

Image not found

Acetic acid, (p-tolyl)-

Measured: 265

Predicted: 270

Image not found

2-Chlorobenzoic acid

Measured: 287

Predicted: 273